



Full wwPDB NMR Structure Validation Report ⓘ

Jun 16, 2024 – 07:03 PM EDT

PDB ID : 5LG9
BMRB ID : 34022
Title : Structure of PfIMP2 (Immune Mapped Protein 2 from Plasmodium falciparum) - an antigenic protein
Authors : Benjamin, S.V.; Matthews, S.J.
Deposited on : 2016-07-06

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

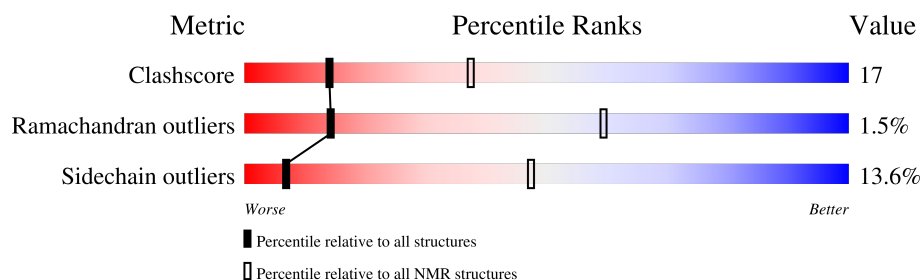
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR


The overall completeness of chemical shifts assignment is 89%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	156	

2 Ensemble composition and analysis

This entry contains 15 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:5-A:90, A:94-A:158 (151)	0.43	2

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	2, 3, 5, 7, 9, 11, 12, 15
2	4, 8, 13, 14
3	1, 6
Single-model clusters	10

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2515 atoms, of which 1277 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

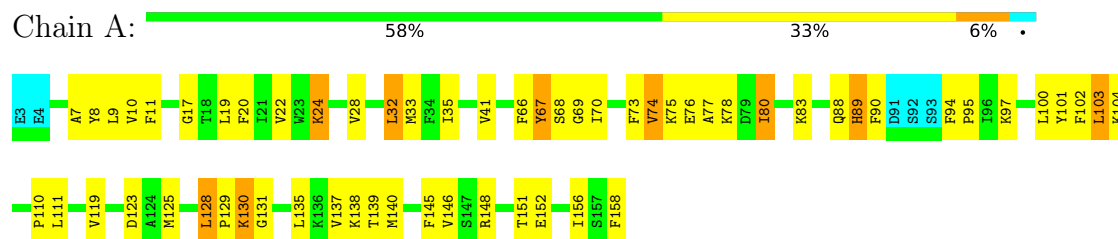
Mol	Chain	Residues	Atoms						Trace
1	A	156	Total	C	H	N	O	S	0
			2515	802	1277	202	228	6	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Uncharacterized protein

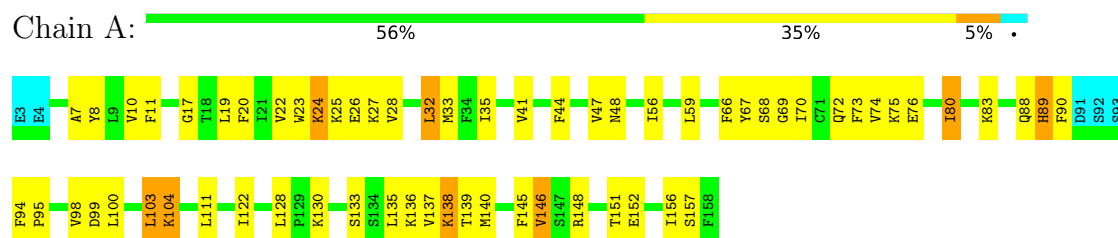


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

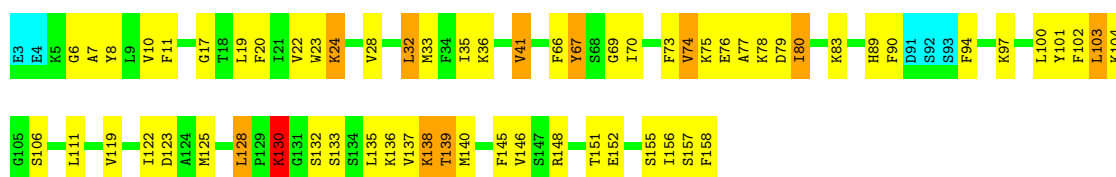
- Molecule 1: Uncharacterized protein



4.2.2 Score per residue for model 2 (medoid)

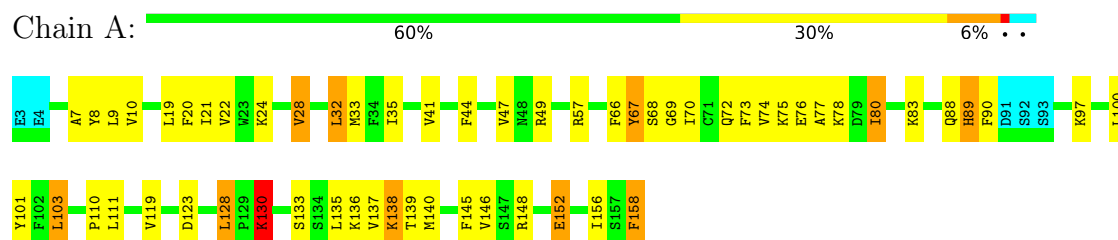
- Molecule 1: Uncharacterized protein





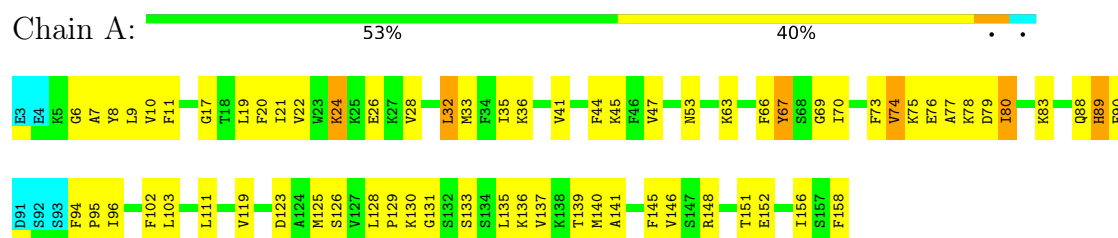
4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein



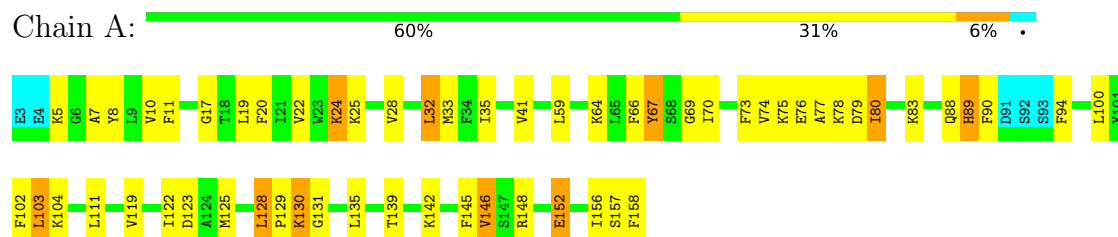
4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized protein



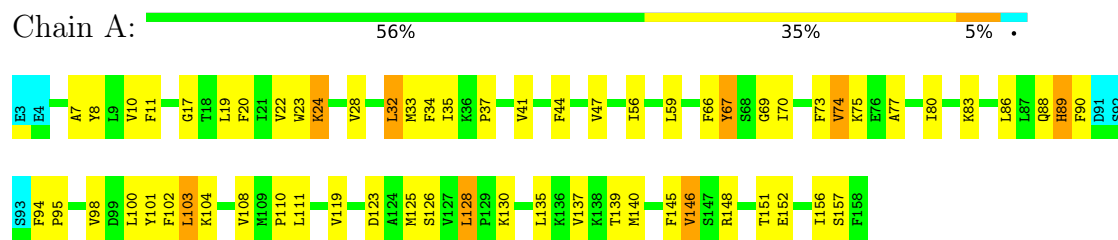
4.2.5 Score per residue for model 5

- Molecule 1: Uncharacterized protein



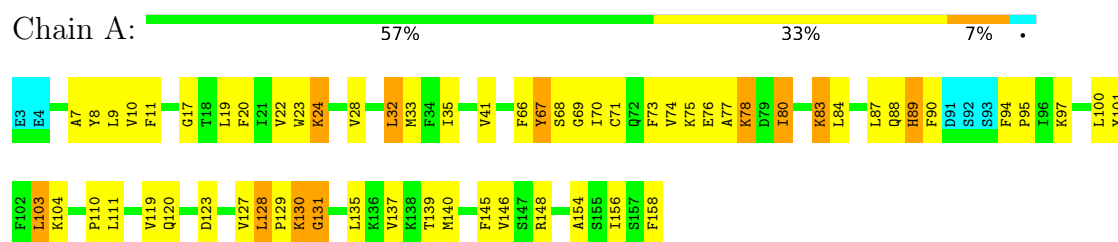
4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized protein



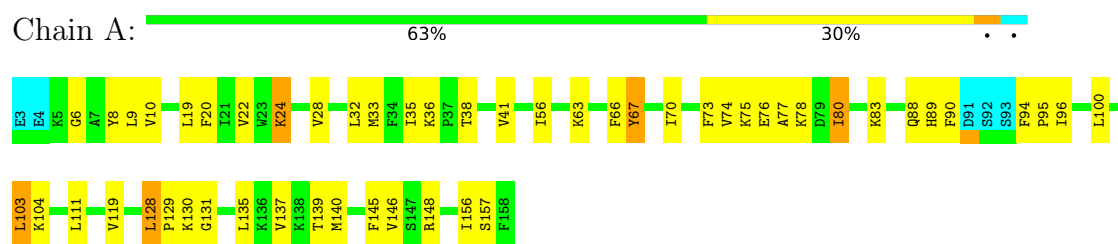
4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized protein



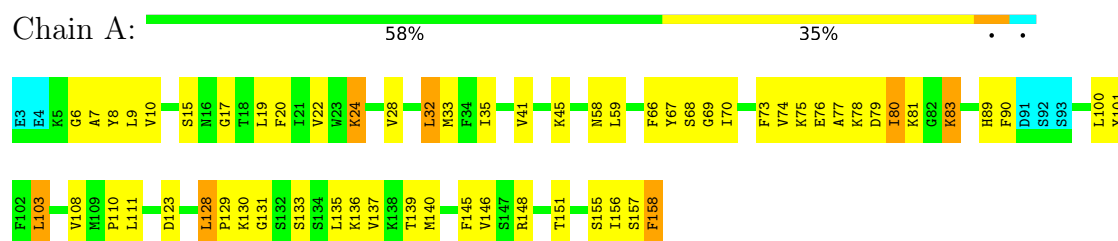
4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein



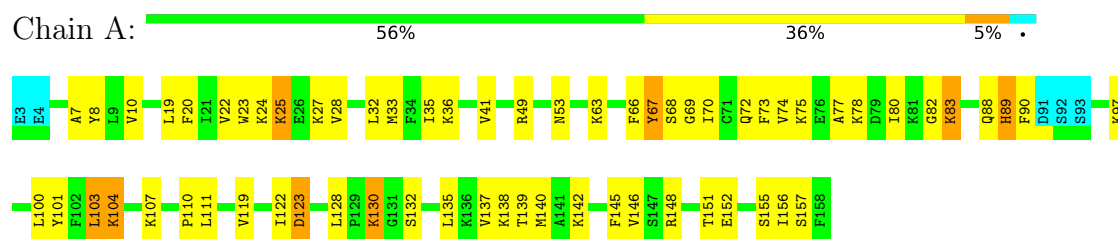
4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein



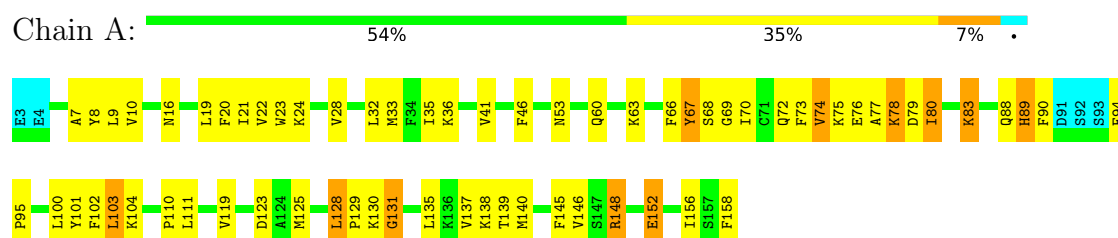
4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein



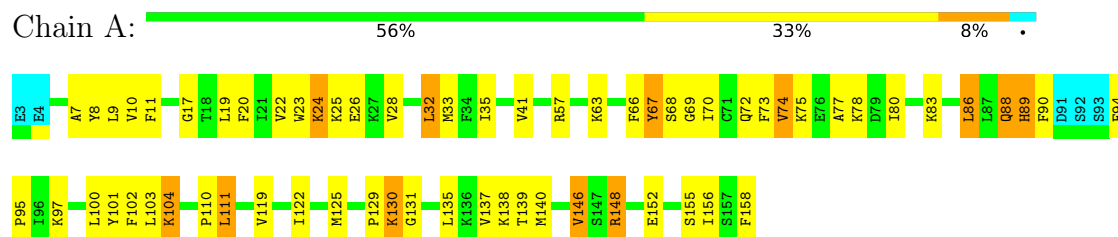
4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized protein



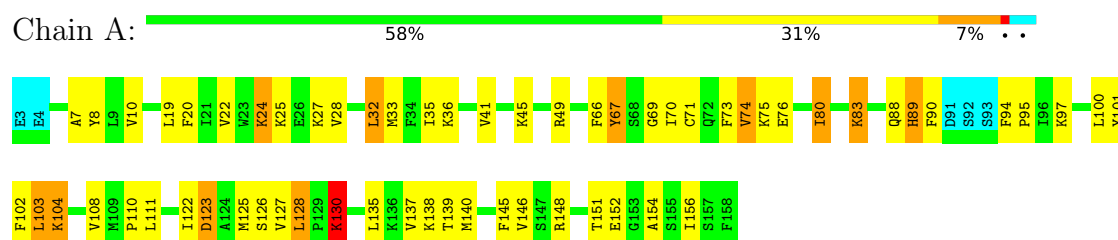
4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein



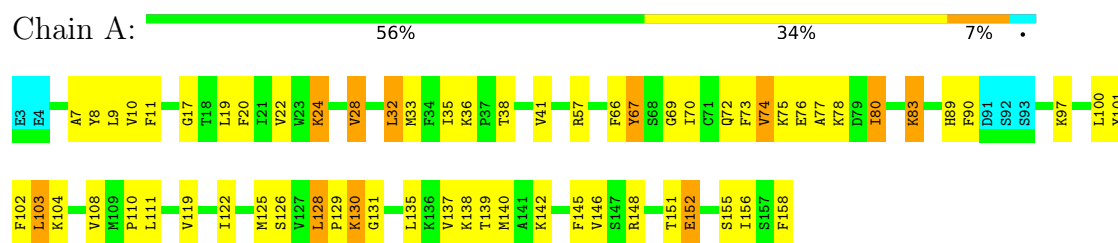
4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized protein



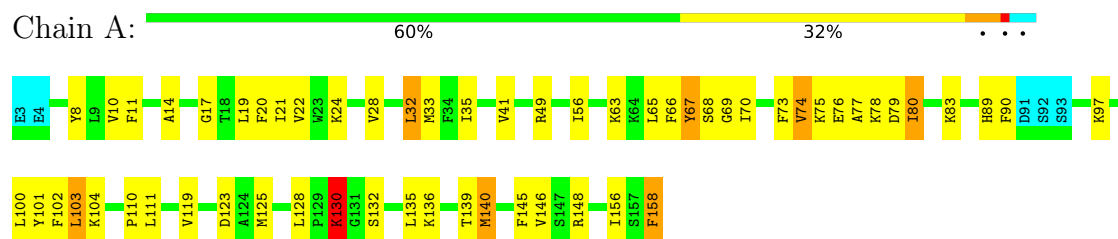
4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized protein



4.2.15 Score per residue for model 15

- Molecule 1: Uncharacterized protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 20 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	refinement	
ARIA	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1925
Number of shifts mapped to atoms	1925
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1200	1249	1248	43±6
All	All	18000	18735	18720	642

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:LYS:HD2	1:A:122:ILE:HG22	0.84	1.49	13	5
1:A:102:PHE:HE1	1:A:125:MET:SD	0.79	1.99	12	9
1:A:74:VAL:HG11	1:A:125:MET:SD	0.75	2.21	15	9
1:A:102:PHE:CE1	1:A:125:MET:SD	0.74	2.80	12	9
1:A:74:VAL:HG21	1:A:125:MET:SD	0.70	2.27	12	9
1:A:24:LYS:HD3	1:A:28:VAL:CG2	0.69	2.17	10	1
1:A:24:LYS:HD2	1:A:28:VAL:HG23	0.69	1.64	6	1
1:A:8:TYR:CD2	1:A:28:VAL:HB	0.68	2.23	9	10
1:A:146:VAL:HA	1:A:155:SER:OG	0.67	1.89	10	5
1:A:137:VAL:CG1	1:A:140:MET:HG3	0.67	2.19	10	12
1:A:146:VAL:HB	1:A:157:SER:OG	0.67	1.89	1	7
1:A:71:CYS:SG	1:A:154:ALA:HB1	0.67	2.29	13	2
1:A:8:TYR:HB2	1:A:22:VAL:CG1	0.67	2.20	6	15
1:A:135:LEU:HD21	1:A:148:ARG:HB2	0.64	1.69	1	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LEU:HG	1:A:90:PHE:CB	0.63	2.23	10	11
1:A:33:MET:SD	1:A:70:ILE:HG23	0.63	2.34	12	15
1:A:78:LYS:HE2	1:A:158:PHE:CE1	0.63	2.29	2	5
1:A:6:GLY:O	1:A:24:LYS:HE3	0.61	1.94	2	4
1:A:137:VAL:CG1	1:A:140:MET:HG2	0.61	2.26	4	1
1:A:24:LYS:N	1:A:24:LYS:HD3	0.60	2.11	5	4
1:A:76:GLU:O	1:A:80:ILE:HG23	0.60	1.97	2	12
1:A:75:LYS:O	1:A:78:LYS:HG2	0.59	1.97	2	4
1:A:77:ALA:HB1	1:A:119:VAL:HG11	0.59	1.73	5	12
1:A:78:LYS:HD2	1:A:158:PHE:CE1	0.59	2.33	5	1
1:A:101:TYR:CZ	1:A:110:PRO:HB3	0.58	2.33	10	10
1:A:19:LEU:HD12	1:A:69:GLY:HA3	0.58	1.75	6	14
1:A:86:LEU:HG	1:A:100:LEU:HD13	0.58	1.74	12	1
1:A:67:TYR:O	1:A:70:ILE:HB	0.58	1.99	12	10
1:A:103:LEU:HD23	1:A:145:PHE:CD2	0.57	2.33	8	12
1:A:22:VAL:HG11	1:A:28:VAL:HG21	0.57	1.75	1	8
1:A:135:LEU:HD22	1:A:140:MET:SD	0.57	2.40	1	5
1:A:86:LEU:HD11	1:A:100:LEU:HD22	0.56	1.76	12	1
1:A:75:LYS:HB2	1:A:156:ILE:CD1	0.55	2.32	11	15
1:A:11:PHE:CE1	1:A:17:GLY:HA2	0.55	2.35	14	9
1:A:135:LEU:HD21	1:A:148:ARG:CB	0.55	2.32	1	9
1:A:7:ALA:HB3	1:A:35:ILE:HB	0.54	1.78	1	13
1:A:104:LYS:CD	1:A:122:ILE:HG22	0.54	2.33	5	3
1:A:97:LYS:O	1:A:130:LYS:HE2	0.54	2.02	3	4
1:A:44:PHE:HA	1:A:47:VAL:HG12	0.54	1.77	1	4
1:A:90:PHE:CE1	1:A:94:PHE:HB2	0.54	2.37	5	2
1:A:44:PHE:HA	1:A:47:VAL:CG1	0.54	2.32	1	4
1:A:21:ILE:HG23	1:A:53:ASN:HB2	0.54	1.79	11	1
1:A:74:VAL:HG11	1:A:125:MET:CE	0.54	2.32	6	7
1:A:128:LEU:HD21	1:A:135:LEU:HD12	0.54	1.79	8	7
1:A:78:LYS:HG2	1:A:119:VAL:HG22	0.53	1.79	12	1
1:A:70:ILE:O	1:A:74:VAL:HG13	0.53	2.02	5	15
1:A:68:SER:O	1:A:72:GLN:HG3	0.53	2.03	1	3
1:A:8:TYR:HB2	1:A:22:VAL:HG12	0.53	1.81	10	1
1:A:16:ASN:O	1:A:60:GLN:HB2	0.53	2.02	11	1
1:A:108:VAL:CG2	1:A:140:MET:HB2	0.53	2.34	6	2
1:A:77:ALA:HA	1:A:80:ILE:CD1	0.52	2.35	9	1
1:A:94:PHE:CD2	1:A:95:PRO:HD2	0.52	2.40	13	2
1:A:22:VAL:CG2	1:A:24:LYS:HD2	0.51	2.36	10	1
1:A:78:LYS:HD2	1:A:158:PHE:CD1	0.51	2.40	15	2
1:A:8:TYR:OH	1:A:27:LYS:HA	0.51	2.06	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:PHE:CG	1:A:95:PRO:HD2	0.50	2.40	7	6
1:A:32:LEU:HG	1:A:90:PHE:CG	0.50	2.40	1	4
1:A:135:LEU:HD13	1:A:145:PHE:CE2	0.50	2.41	4	4
1:A:101:TYR:CE1	1:A:132:SER:HB2	0.50	2.41	15	2
1:A:148:ARG:O	1:A:151:THR:HG22	0.50	2.07	1	8
1:A:103:LEU:HD12	1:A:123:ASP:HB2	0.50	1.83	4	8
1:A:88:GLN:O	1:A:89:HIS:HB2	0.50	2.06	1	10
1:A:7:ALA:HA	1:A:22:VAL:O	0.49	2.07	4	6
1:A:35:ILE:HG13	1:A:73:PHE:CZ	0.49	2.42	6	15
1:A:130:LYS:HA	1:A:130:LYS:HE2	0.49	1.85	14	6
1:A:97:LYS:C	1:A:130:LYS:HE3	0.49	2.28	7	3
1:A:66:PHE:O	1:A:70:ILE:HG13	0.49	2.08	1	15
1:A:102:PHE:CD1	1:A:125:MET:HB2	0.49	2.43	14	7
1:A:56:ILE:HG23	1:A:59:LEU:HD21	0.49	1.84	1	2
1:A:129:PRO:O	1:A:131:GLY:N	0.48	2.47	12	8
1:A:125:MET:HG3	1:A:126:SER:N	0.48	2.23	4	4
1:A:49:ARG:HD2	1:A:53:ASN:OD1	0.48	2.08	10	1
1:A:78:LYS:HD3	1:A:158:PHE:CE1	0.47	2.44	12	1
1:A:100:LEU:N	1:A:100:LEU:HD12	0.47	2.25	5	13
1:A:123:ASP:O	1:A:158:PHE:HB2	0.47	2.10	3	1
1:A:24:LYS:HE2	1:A:28:VAL:HG13	0.47	1.85	14	1
1:A:23:TRP:CZ3	1:A:41:VAL:HG11	0.47	2.44	2	1
1:A:138:LYS:HD2	1:A:138:LYS:H	0.47	1.69	2	1
1:A:45:LYS:O	1:A:49:ARG:HB2	0.47	2.10	13	1
1:A:8:TYR:CD2	1:A:28:VAL:HG22	0.46	2.45	14	2
1:A:133:SER:HA	1:A:136:LYS:HB3	0.46	1.87	1	4
1:A:83:LYS:HD2	1:A:83:LYS:N	0.46	2.26	13	6
1:A:63:LYS:HD2	1:A:96:ILE:HG12	0.46	1.87	8	1
1:A:7:ALA:O	1:A:34:PHE:HA	0.46	2.11	6	1
1:A:7:ALA:HB2	1:A:23:TRP:CZ3	0.45	2.46	2	6
1:A:32:LEU:HG	1:A:90:PHE:HB3	0.45	1.87	6	9
1:A:74:VAL:HG23	1:A:78:LYS:NZ	0.45	2.26	5	1
1:A:100:LEU:HD23	1:A:125:MET:HE1	0.45	1.87	6	3
1:A:75:LYS:HA	1:A:78:LYS:HD3	0.45	1.89	8	3
1:A:102:PHE:CE1	1:A:125:MET:HB2	0.45	2.46	5	3
1:A:24:LYS:HD3	1:A:24:LYS:H	0.45	1.70	5	2
1:A:108:VAL:HG21	1:A:135:LEU:O	0.45	2.11	14	2
1:A:9:LEU:HD23	1:A:73:PHE:CD2	0.45	2.47	4	7
1:A:24:LYS:HG3	1:A:26:GLU:O	0.45	2.12	4	1
1:A:24:LYS:HG2	1:A:26:GLU:H	0.45	1.72	1	1
1:A:19:LEU:HD11	1:A:66:PHE:HD1	0.44	1.72	15	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LEU:HD23	1:A:66:PHE:CZ	0.44	2.46	4	2
1:A:141:ALA:O	1:A:145:PHE:HB2	0.44	2.11	4	1
1:A:137:VAL:HG22	1:A:138:LYS:N	0.44	2.26	3	6
1:A:32:LEU:CD1	1:A:32:LEU:N	0.44	2.81	6	2
1:A:23:TRP:HB3	1:A:46:PHE:CE2	0.44	2.48	11	1
1:A:67:TYR:CD1	1:A:67:TYR:N	0.44	2.86	10	4
1:A:104:LYS:HD3	1:A:122:ILE:HG22	0.44	1.89	5	1
1:A:9:LEU:CB	1:A:33:MET:HB2	0.44	2.42	8	2
1:A:19:LEU:HD21	1:A:66:PHE:CD1	0.44	2.48	15	2
1:A:86:LEU:HD21	1:A:111:LEU:HG	0.44	1.90	12	1
1:A:128:LEU:HD12	1:A:152:GLU:HG3	0.44	1.89	2	1
1:A:125:MET:CG	1:A:126:SER:N	0.43	2.81	4	4
1:A:44:PHE:CE2	1:A:48:ASN:HB2	0.43	2.48	1	1
1:A:77:ALA:CB	1:A:119:VAL:HG11	0.43	2.43	10	5
1:A:128:LEU:HD12	1:A:152:GLU:CB	0.43	2.42	11	3
1:A:32:LEU:HG	1:A:90:PHE:HB2	0.43	1.89	11	2
1:A:100:LEU:HB3	1:A:125:MET:HE2	0.43	1.90	12	1
1:A:21:ILE:CD1	1:A:76:GLU:HG3	0.43	2.44	3	3
1:A:88:GLN:OE1	1:A:88:GLN:HA	0.43	2.13	8	1
1:A:78:LYS:HB2	1:A:78:LYS:NZ	0.43	2.28	15	1
1:A:63:LYS:HD2	1:A:96:ILE:CG1	0.43	2.43	8	1
1:A:35:ILE:HG13	1:A:73:PHE:CE1	0.43	2.49	3	2
1:A:64:LYS:HA	1:A:67:TYR:CD1	0.43	2.49	5	1
1:A:19:LEU:HB2	1:A:56:ILE:HG22	0.43	1.91	8	1
1:A:107:LYS:HD3	1:A:138:LYS:O	0.43	2.14	10	1
1:A:101:TYR:OH	1:A:136:LYS:HE2	0.43	2.14	15	1
1:A:106:SER:O	1:A:139:THR:HG22	0.42	2.14	2	1
1:A:83:LYS:HE3	1:A:120:GLN:OE1	0.42	2.14	7	1
1:A:140:MET:SD	1:A:145:PHE:HD2	0.42	2.37	15	1
1:A:17:GLY:O	1:A:59:LEU:HG	0.42	2.14	5	2
1:A:142:LYS:O	1:A:146:VAL:HG12	0.42	2.13	5	3
1:A:24:LYS:HD2	1:A:28:VAL:CG2	0.42	2.41	6	2
1:A:71:CYS:SG	1:A:127:VAL:HG23	0.42	2.53	7	2
1:A:68:SER:O	1:A:72:GLN:HG2	0.42	2.13	12	2
1:A:70:ILE:HG21	1:A:100:LEU:HD21	0.42	1.91	12	1
1:A:25:LYS:N	1:A:25:LYS:HD3	0.42	2.30	10	1
1:A:104:LYS:HE2	1:A:122:ILE:HG22	0.42	1.92	12	1
1:A:98:VAL:HB	1:A:128:LEU:O	0.42	2.14	1	2
1:A:67:TYR:N	1:A:67:TYR:CD1	0.42	2.88	8	3
1:A:56:ILE:HD13	1:A:65:LEU:O	0.42	2.15	15	1
1:A:75:LYS:HA	1:A:78:LYS:HE3	0.42	1.92	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:PHE:CE1	1:A:122:ILE:HD13	0.42	2.50	12	1
1:A:32:LEU:N	1:A:32:LEU:CD1	0.42	2.82	5	2
1:A:15:SER:O	1:A:58:ASN:HA	0.42	2.15	9	1
1:A:137:VAL:HG13	1:A:140:MET:HG3	0.41	1.91	2	1
1:A:78:LYS:HD3	1:A:158:PHE:CD1	0.41	2.50	12	1
1:A:133:SER:HA	1:A:136:LYS:CB	0.41	2.45	2	2
1:A:8:TYR:HD2	1:A:24:LYS:CE	0.41	2.28	7	1
1:A:135:LEU:HD13	1:A:145:PHE:CD2	0.41	2.51	4	2
1:A:97:LYS:O	1:A:130:LYS:HE3	0.41	2.16	12	1
1:A:74:VAL:HG11	1:A:125:MET:HE1	0.41	1.90	5	2
1:A:33:MET:HG2	1:A:86:LEU:HD12	0.41	1.92	6	1
1:A:130:LYS:HE2	1:A:130:LYS:CA	0.41	2.46	10	1
1:A:99:ASP:OD2	1:A:130:LYS:HE2	0.41	2.16	1	1
1:A:24:LYS:HE3	1:A:24:LYS:H	0.41	1.76	6	1
1:A:32:LEU:O	1:A:87:LEU:HB2	0.41	2.16	7	1
1:A:82:GLY:C	1:A:83:LYS:HD2	0.41	2.35	10	1
1:A:100:LEU:HB3	1:A:125:MET:CE	0.41	2.45	11	1
1:A:63:LYS:HE2	1:A:96:ILE:HG12	0.41	1.93	4	1
1:A:128:LEU:HG	1:A:152:GLU:HG2	0.41	1.93	5	1
1:A:72:GLN:O	1:A:75:LYS:HB3	0.41	2.16	14	1
1:A:140:MET:SD	1:A:145:PHE:HB2	0.41	2.56	15	1
1:A:19:LEU:HD11	1:A:66:PHE:CD1	0.41	2.50	3	3
1:A:33:MET:CE	1:A:84:LEU:HD11	0.41	2.46	7	1
1:A:37:PRO:CB	1:A:41:VAL:HB	0.40	2.46	6	1
1:A:86:LEU:HD22	1:A:86:LEU:N	0.40	2.32	12	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	150/156 (96%)	138±2 (92±1%)	10±2 (7±1%)	2±1 (1±0%)	14	59
All	All	2250/2340 (96%)	2065 (92%)	152 (7%)	33 (1%)	14	59

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	89	HIS	15
1	A	130	LYS	14
1	A	131	GLY	2
1	A	81	LYS	1
1	A	14	ALA	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	134/139 (96%)	116±2 (86±2%)	18±2 (14±2%)	7	47
All	All	2010/2085 (96%)	1737 (86%)	273 (14%)	7	47

All 39 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	10	VAL	15
1	A	20	PHE	15
1	A	67	TYR	15
1	A	80	ILE	15
1	A	111	LEU	15
1	A	139	THR	15
1	A	24	LYS	14
1	A	41	VAL	14
1	A	83	LYS	14
1	A	103	LEU	14
1	A	128	LEU	13
1	A	32	LEU	12
1	A	146	VAL	10
1	A	152	GLU	10
1	A	104	LYS	9
1	A	74	VAL	8
1	A	36	LYS	7
1	A	79	ASP	6
1	A	25	LYS	5
1	A	130	LYS	4
1	A	158	PHE	4

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Mol	Chain	Res	Type	Models (Total)
1	A	123	ASP	4
1	A	63	LYS	4
1	A	138	LYS	3
1	A	28	VAL	3
1	A	57	ARG	3
1	A	68	SER	3
1	A	78	LYS	3
1	A	27	LYS	2
1	A	49	ARG	2
1	A	45	LYS	2
1	A	38	THR	2
1	A	148	ARG	2
1	A	53	ASN	1
1	A	5	LYS	1
1	A	132	SER	1
1	A	86	LEU	1
1	A	88	GLN	1
1	A	140	MET	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 89% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1925
Number of shifts mapped to atoms	1925
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	236

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	156	-0.21 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	146	-0.10 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	151	0.17 ± 0.10	None needed (< 0.5 ppm)
^{15}N	144	0.09 ± 0.38	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 89%, i.e. 1881 atoms were assigned a chemical shift out of a possible 2118. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	739/753 (98%)	301/306 (98%)	298/302 (99%)	140/145 (97%)
Sidechain	1063/1188 (89%)	723/772 (94%)	340/373 (91%)	0/43 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	79/177 (45%)	40/87 (46%)	38/87 (44%)	1/3 (33%)
Overall	1881/2118 (89%)	1064/1165 (91%)	676/762 (89%)	141/191 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 1924 atoms were assigned a chemical shift out of a possible 2167. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	761/778 (98%)	310/316 (98%)	307/312 (98%)	144/150 (96%)
Sidechain	1084/1212 (89%)	737/786 (94%)	347/383 (91%)	0/43 (0%)
Aromatic	79/177 (45%)	40/87 (46%)	38/87 (44%)	1/3 (33%)
Overall	1924/2167 (89%)	1087/1189 (91%)	692/782 (88%)	145/196 (74%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	90	PHE	CD1	35.19	125.33 – 137.83	-77.1
1	A	11	PHE	CD1	35.73	125.33 – 137.83	-76.7
1	A	20	PHE	CD1	35.73	125.33 – 137.83	-76.7
1	A	73	PHE	CD1	35.73	125.33 – 137.83	-76.7
1	A	34	PHE	CD1	35.85	125.33 – 137.83	-76.6
1	A	44	PHE	CD1	35.95	125.33 – 137.83	-76.5
1	A	117	PHE	CD1	35.95	125.33 – 137.83	-76.5
1	A	145	PHE	CD1	35.95	125.33 – 137.83	-76.5
1	A	158	PHE	CD1	35.95	125.33 – 137.83	-76.5
1	A	66	PHE	CD1	36.05	125.33 – 137.83	-76.4
1	A	102	PHE	CD1	36.15	125.33 – 137.83	-76.3
1	A	94	PHE	CD1	36.23	125.33 – 137.83	-76.3
1	A	46	PHE	CD1	36.35	125.33 – 137.83	-76.2
1	A	20	PHE	CE1	32.48	124.17 – 137.29	-74.9
1	A	11	PHE	CE1	33.45	124.17 – 137.29	-74.1
1	A	158	PHE	CE1	34.23	124.17 – 137.29	-73.5
1	A	90	PHE	CE1	35.23	124.17 – 137.29	-72.8
1	A	44	PHE	CE1	35.65	124.17 – 137.29	-72.5
1	A	117	PHE	CE1	35.73	124.17 – 137.29	-72.4
1	A	34	PHE	CE1	35.85	124.17 – 137.29	-72.3
1	A	145	PHE	CE1	35.95	124.17 – 137.29	-72.2
1	A	46	PHE	CE1	35.98	124.17 – 137.29	-72.2

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	66	PHE	CE1	36.15	124.17 – 137.29	-72.1
1	A	102	PHE	CE1	36.15	124.17 – 137.29	-72.1
1	A	8	TYR	CD1	35.47	125.84 – 139.60	-70.7
1	A	101	TYR	CD1	35.95	125.84 – 139.60	-70.3
1	A	67	TYR	CD1	36.48	125.84 – 139.60	-69.9
1	A	46	PHE	CZ	33.23	121.82 – 136.66	-64.7
1	A	23	TRP	CH2	26.65	116.19 – 131.43	-63.8
1	A	34	PHE	CZ	35.75	121.82 – 136.66	-63.0
1	A	23	TRP	CD1	30.42	117.34 – 135.80	-52.1
1	A	67	TYR	CE1	53.84	111.24 – 124.66	-47.8
1	A	8	TYR	CE1	54.67	111.24 – 124.66	-47.2
1	A	101	TYR	CE1	54.67	111.24 – 124.66	-47.2
1	A	23	TRP	CZ2	50.24	107.20 – 121.33	-45.3
1	A	23	TRP	CZ3	56.34	113.48 – 129.28	-41.2
1	A	89	HIS	CE1	42.98	126.08 – 149.12	-41.1
1	A	23	TRP	CE3	56.47	111.58 – 129.41	-35.9
1	A	85	THR	CG2	54.19	16.06 – 27.03	29.8
1	A	5	LYS	CG	57.71	19.35 – 30.45	29.6
1	A	52	LYS	CG	57.71	19.35 – 30.45	29.6
1	A	36	LYS	CG	57.70	19.35 – 30.45	29.6
1	A	64	LYS	CG	57.69	19.35 – 30.45	29.6
1	A	81	LYS	CG	57.47	19.35 – 30.45	29.3
1	A	63	LYS	CG	57.44	19.35 – 30.45	29.3
1	A	104	LYS	CG	57.40	19.35 – 30.45	29.3
1	A	75	LYS	CG	57.38	19.35 – 30.45	29.3
1	A	151	THR	CG2	53.57	16.06 – 27.03	29.2
1	A	38	THR	CG2	53.56	16.06 – 27.03	29.2
1	A	78	LYS	CG	57.28	19.35 – 30.45	29.2
1	A	138	LYS	CG	57.27	19.35 – 30.45	29.2
1	A	113	THR	CG2	53.53	16.06 – 27.03	29.1
1	A	136	LYS	CG	57.25	19.35 – 30.45	29.1
1	A	139	THR	CG2	53.48	16.06 – 27.03	29.1
1	A	107	LYS	CG	57.18	19.35 – 30.45	29.1
1	A	142	LYS	CG	57.13	19.35 – 30.45	29.0
1	A	18	THR	CG2	53.32	16.06 – 27.03	29.0
1	A	97	LYS	CG	56.80	19.35 – 30.45	28.7
1	A	59	LEU	CG	57.73	21.37 – 32.19	28.6
1	A	39	LYS	CG	56.54	19.35 – 30.45	28.5
1	A	130	LYS	CG	55.55	19.35 – 30.45	27.6
1	A	81	LYS	CD	57.57	23.50 – 34.42	26.2
1	A	122	ILE	CG2	51.65	10.93 – 24.12	25.9
1	A	74	VAL	CG1	55.95	14.71 – 28.29	25.4

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	45	LYS	CD	56.58	23.50 – 34.42	25.3
1	A	70	ILE	CG2	50.53	10.93 – 24.12	25.0
1	A	96	ILE	CG2	50.50	10.93 – 24.12	25.0
1	A	35	ILE	CG2	50.23	10.93 – 24.12	24.8
1	A	98	VAL	CG1	54.82	14.71 – 28.29	24.5
1	A	146	VAL	CG1	54.78	14.71 – 28.29	24.5
1	A	57	ARG	CG	56.50	21.24 – 33.19	24.5
1	A	108	VAL	CG1	54.52	14.71 – 28.29	24.3
1	A	56	ILE	CG2	49.45	10.93 – 24.12	24.2
1	A	80	ILE	CG2	49.44	10.93 – 24.12	24.2
1	A	127	VAL	CG1	54.09	14.71 – 28.29	24.0
1	A	22	VAL	CG1	53.94	14.71 – 28.29	23.9
1	A	21	ILE	CG2	49.01	10.93 – 24.12	23.9
1	A	119	VAL	CG1	53.66	14.71 – 28.29	23.7
1	A	28	VAL	CG1	53.39	14.71 – 28.29	23.5
1	A	10	VAL	CG1	53.33	14.71 – 28.29	23.4
1	A	118	VAL	CG1	53.31	14.71 – 28.29	23.4
1	A	47	VAL	CG1	53.29	14.71 – 28.29	23.4
1	A	41	VAL	CG1	53.23	14.71 – 28.29	23.4
1	A	156	ILE	CG2	48.29	10.93 – 24.12	23.3
1	A	15	SER	CB	29.20	56.28 – 71.32	-23.0
1	A	110	PRO	CA	30.05	55.85 – 70.84	-22.2
1	A	68	SER	CB	30.47	56.28 – 71.32	-22.2
1	A	137	VAL	CG1	51.41	14.71 – 28.29	22.0
1	A	119	VAL	CG2	54.68	13.71 – 28.88	22.0
1	A	74	VAL	CG2	54.58	13.71 – 28.88	21.9
1	A	108	VAL	CG2	54.50	13.71 – 28.88	21.9
1	A	147	SER	CB	30.88	56.28 – 71.32	-21.9
1	A	134	SER	CB	30.94	56.28 – 71.32	-21.9
1	A	132	SER	CB	31.15	56.28 – 71.32	-21.7
1	A	22	VAL	CG2	54.06	13.71 – 28.88	21.6
1	A	42	PRO	CA	30.97	55.85 – 70.84	-21.6
1	A	127	VAL	CG2	54.06	13.71 – 28.88	21.6
1	A	28	VAL	CG2	54.02	13.71 – 28.88	21.6
1	A	10	VAL	CG2	53.95	13.71 – 28.88	21.5
1	A	37	PRO	CA	31.08	55.85 – 70.84	-21.5
1	A	129	PRO	CA	31.08	55.85 – 70.84	-21.5
1	A	116	PRO	CA	31.26	55.85 – 70.84	-21.4
1	A	137	VAL	CG2	53.77	13.71 – 28.88	21.4
1	A	133	SER	CB	31.94	56.28 – 71.32	-21.2
1	A	61	SER	CB	31.99	56.28 – 71.32	-21.1
1	A	118	VAL	CG2	53.34	13.71 – 28.88	21.1

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	47	VAL	CG2	53.29	13.71 – 28.88	21.1
1	A	154	ALA	CB	55.96	10.19 – 27.75	21.1
1	A	41	VAL	CG2	53.23	13.71 – 28.88	21.1
1	A	146	VAL	CG2	53.12	13.71 – 28.88	21.0
1	A	92	SER	CB	32.40	56.28 – 71.32	-20.9
1	A	65	LEU	CD1	57.60	16.71 – 32.55	20.8
1	A	100	LEU	CD1	57.53	16.71 – 32.55	20.8
1	A	19	LEU	CD1	57.49	16.71 – 32.55	20.8
1	A	106	SER	CB	32.59	56.28 – 71.32	-20.8
1	A	157	SER	CB	32.97	56.28 – 71.32	-20.5
1	A	56	ILE	CD1	46.91	5.18 – 21.60	20.4
1	A	156	ILE	CD1	46.82	5.18 – 21.60	20.4
1	A	93	SER	CB	33.19	56.28 – 71.32	-20.4
1	A	122	ILE	CD1	46.60	5.18 – 21.60	20.2
1	A	124	ALA	CB	54.24	10.19 – 27.75	20.1
1	A	80	ILE	CD1	46.36	5.18 – 21.60	20.1
1	A	59	LEU	CD2	57.70	15.73 – 32.47	20.1
1	A	95	PRO	CA	33.29	55.85 – 70.84	-20.1
1	A	111	LEU	CD1	56.35	16.71 – 32.55	20.0
1	A	21	ILE	CD1	46.01	5.18 – 21.60	19.9
1	A	55	LEU	CD1	55.80	16.71 – 32.55	19.7
1	A	31	ALA	CB	53.46	10.19 – 27.75	19.6
1	A	128	LEU	CD1	55.71	16.71 – 32.55	19.6
1	A	84	LEU	CD2	56.67	15.73 – 32.47	19.5
1	A	135	LEU	CD2	56.61	15.73 – 32.47	19.4
1	A	70	ILE	CD1	45.26	5.18 – 21.60	19.4
1	A	9	LEU	CD1	55.35	16.71 – 32.55	19.4
1	A	98	VAL	CG2	50.71	13.71 – 28.88	19.4
1	A	103	LEU	CD1	55.21	16.71 – 32.55	19.3
1	A	113	THR	CB	36.74	61.12 – 78.27	-19.2
1	A	33	MET	CE	50.48	8.39 – 25.85	19.1
1	A	35	ILE	CD1	44.63	5.18 – 21.60	19.0
1	A	96	ILE	CD1	44.58	5.18 – 21.60	19.0
1	A	32	LEU	CD2	55.79	15.73 – 32.47	18.9
1	A	151	THR	CB	37.24	61.12 – 78.27	-18.9
1	A	55	LEU	CD2	55.70	15.73 – 32.47	18.9
1	A	155	SER	CB	35.54	56.28 – 71.32	-18.8
1	A	141	ALA	CB	51.88	10.19 – 27.75	18.7
1	A	38	THR	CB	37.59	61.12 – 78.27	-18.7
1	A	9	LEU	CD2	55.38	15.73 – 32.47	18.7
1	A	144	MET	CE	49.72	8.39 – 25.85	18.7
1	A	126	SER	CB	35.75	56.28 – 71.32	-18.6

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	103	LEU	CD2	55.24	15.73 – 32.47	18.6
1	A	7	ALA	CB	51.51	10.19 – 27.75	18.5
1	A	14	ALA	CB	51.49	10.19 – 27.75	18.5
1	A	32	LEU	CD1	53.79	16.71 – 32.55	18.4
1	A	19	LEU	CD2	54.79	15.73 – 32.47	18.3
1	A	65	LEU	CD2	54.61	15.73 – 32.47	18.2
1	A	87	LEU	CD2	54.33	15.73 – 32.47	18.1
1	A	77	ALA	CB	50.17	10.19 – 27.75	17.8
1	A	85	THR	CB	39.61	61.12 – 78.27	-17.5
1	A	122	ILE	CG1	57.58	19.24 – 36.26	17.5
1	A	139	THR	CB	40.39	61.12 – 78.27	-17.1
1	A	18	THR	CB	41.11	61.12 – 78.27	-16.7
1	A	106	SER	CA	25.80	48.46 – 68.96	-16.1
1	A	126	SER	CA	26.48	48.46 – 68.96	-15.7
1	A	133	SER	CA	26.99	48.46 – 68.96	-15.5
1	A	132	SER	CA	27.37	48.46 – 68.96	-15.3
1	A	93	SER	CA	27.39	48.46 – 68.96	-15.3
1	A	29	GLU	CA	25.99	47.03 – 67.62	-15.2
1	A	3	GLU	CA	26.08	47.03 – 67.62	-15.2
1	A	61	SER	CA	27.75	48.46 – 68.96	-15.1
1	A	54	GLU	CA	26.34	47.03 – 67.62	-15.1
1	A	43	GLU	CA	26.78	47.03 – 67.62	-14.8
1	A	60	GLN	CA	25.75	46.17 – 66.97	-14.8
1	A	92	SER	CA	28.89	48.46 – 68.96	-14.6
1	A	76	GLU	CA	27.43	47.03 – 67.62	-14.5
1	A	147	SER	CA	29.48	48.46 – 68.96	-14.3
1	A	72	GLN	CA	26.95	46.17 – 66.97	-14.2
1	A	134	SER	CA	29.55	48.46 – 68.96	-14.2
1	A	59	LEU	CA	26.08	45.17 – 66.21	-14.1
1	A	138	LYS	CA	26.68	46.18 – 67.77	-14.0
1	A	144	MET	CA	25.73	45.26 – 67.07	-14.0
1	A	139	THR	CA	26.85	49.41 – 75.05	-13.8
1	A	68	SER	CA	30.47	48.46 – 68.96	-13.8
1	A	49	ARG	CA	25.72	45.44 – 68.13	-13.7
1	A	64	LYS	CA	27.46	46.18 – 67.77	-13.7
1	A	78	LYS	CA	27.48	46.18 – 67.77	-13.7
1	A	63	LYS	CA	27.66	46.18 – 67.77	-13.6
1	A	142	LYS	CA	28.43	46.18 – 67.77	-13.2
1	A	75	LYS	CA	28.62	46.18 – 67.77	-13.1
1	A	148	ARG	CA	27.22	45.44 – 68.13	-13.0
1	A	35	ILE	CA	27.32	48.30 – 75.08	-12.8
1	A	18	THR	CA	29.59	49.41 – 75.05	-12.7

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	90	PHE	CA	25.84	45.38 – 70.89	-12.7
1	A	85	THR	CA	29.85	49.41 – 75.05	-12.6
1	A	56	ILE	CA	27.92	48.30 – 75.08	-12.6
1	A	41	VAL	CA	26.85	48.38 – 76.73	-12.6
1	A	98	VAL	CA	26.95	48.38 – 76.73	-12.6
1	A	89	HIS	CA	27.82	45.04 – 67.94	-12.5
1	A	156	ILE	CA	28.22	48.30 – 75.08	-12.5
1	A	23	TRP	CE2	56.42	105.29 – 170.61	-12.5
1	A	122	ILE	CA	28.32	48.30 – 75.08	-12.5
1	A	96	ILE	CA	28.34	48.30 – 75.08	-12.4
1	A	137	VAL	CA	27.31	48.38 – 76.73	-12.4
1	A	67	TYR	CA	27.33	45.75 – 70.63	-12.4
1	A	80	ILE	CA	28.60	48.30 – 75.08	-12.3
1	A	21	ILE	CA	28.63	48.30 – 75.08	-12.3
1	A	38	THR	CA	30.65	49.41 – 75.05	-12.3
1	A	158	PHE	CA	27.12	45.38 – 70.89	-12.2
1	A	46	PHE	CA	27.21	45.38 – 70.89	-12.1
1	A	127	VAL	CA	28.19	48.38 – 76.73	-12.1
1	A	22	VAL	CA	28.29	48.38 – 76.73	-12.1
1	A	28	VAL	CA	28.89	48.38 – 76.73	-11.9
1	A	10	VAL	CA	29.06	48.38 – 76.73	-11.8
1	A	44	PHE	CA	28.26	45.38 – 70.89	-11.7
1	A	119	VAL	CA	29.77	48.38 – 76.73	-11.6
1	A	113	THR	CA	33.00	49.41 – 75.05	-11.4
1	A	108	VAL	CA	30.64	48.38 – 76.73	-11.3
1	A	151	THR	CA	33.90	49.41 – 75.05	-11.1
1	A	145	PHE	CA	30.06	45.38 – 70.89	-11.0
1	A	66	PHE	CA	30.15	45.38 – 70.89	-11.0
1	A	118	VAL	CA	31.61	48.38 – 76.73	-10.9
1	A	73	PHE	CA	30.43	45.38 – 70.89	-10.9
1	A	47	VAL	CA	31.94	48.38 – 76.73	-10.8
1	A	70	ILE	CA	32.87	48.30 – 75.08	-10.8
1	A	146	VAL	CA	33.42	48.38 – 76.73	-10.3
1	A	74	VAL	CA	35.13	48.38 – 76.73	-9.7
1	A	140	MET	CE	32.50	8.39 – 25.85	8.8
1	A	71	CYS	CA	32.31	40.80 – 75.33	-7.5
1	A	7	ALA	HB1	-0.36	0.14 – 2.58	-7.0
1	A	7	ALA	HB2	-0.36	0.14 – 2.58	-7.0
1	A	7	ALA	HB3	-0.36	0.14 – 2.58	-7.0
1	A	45	LYS	HB3	0.03	0.46 – 3.04	-6.7
1	A	45	LYS	HD3	0.21	0.54 – 2.65	-6.6
1	A	95	PRO	HD2	1.45	1.93 – 5.38	-6.4

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	82	GLY	N	131.04	91.59 – 127.52	6.0
1	A	51	GLY	N	130.25	91.59 – 127.52	5.8
1	A	149	GLY	N	130.26	91.59 – 127.52	5.8
1	A	45	LYS	HD2	0.48	0.58 – 2.64	-5.5

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

